MONTE CARLO CALCULATIONS OF ELEMENTARY PARTICLE PROPERTIES

G. S. GURALNIK
BROWN UNIVERSITY
PROVIDENCE, RHODE ISLAND

TONY WARNOCK
CRAY RESEARCH
MINNEAPOLIS, MINNESOTA

AND

CHARLES ZEMACH
LOS ALAMOS NATIONAL LABORATORY
LOS ALAMOS, NEW MEXICO

MONTE CARLO CALCULATIONS OF ELEMENTARY PARTICLE PROPERTIES

G.S. Guralnik
Brown University and Los Alamos National Laboratory

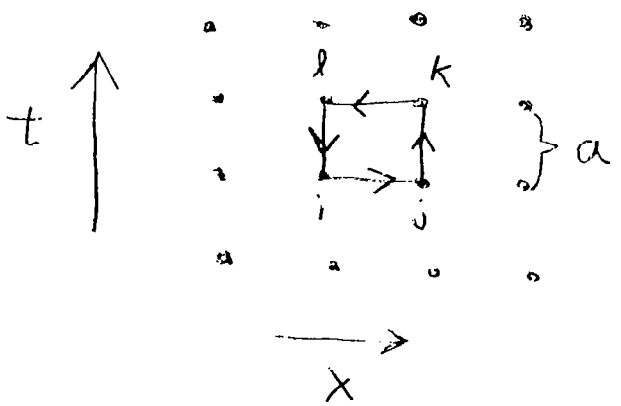
Tony Warnock
Cray Research

Charles Zemach
Los Alamos National Laboratory

The object of our project is to calculate the masses of the "elementary particles". This ambitious goal apparently is not possible using analytic methods or known approximation methods. However, it is probable that the power of a modern super computer will make at least part of the low lying mass spectrum accessible through direct numerical computation. Initial attempts by several groups at calculating this spectrum on small lattices of space time points have been very promising. Using new methods and super computers we have made considerable progress towards evaluating the mass spectrum on comparatively large lattices. Even so, we are examining regions of space just barely large enough to contain the particles being examined. Only more time and faster machines with increased storage will allow calculations of systems with guaranteed minimal boundary effects. In what follows we outline the ideas that currently go into this calculation

While a long time ago it was believed that there were only a relatively small number of such objects (for example, protons, neutrons,electrons, photons and so on) it is now known that there is a virtual alphabet soup of so called elementary particles. A partial listing of these in terms of standardized short hand description is: $\pi^{\pm}$, π^{0}, η, $K^{\pm}$, K^{0}, $\bar{K}^{0}$, $D^{\pm}$, D^{0}, $\bar{D}^{0}$, $F^{\pm}$, P, N, Λ, $\Sigma^{\pm}$, Ξ^{0} Ξ^{-} Ω^{-} γ ν_{e}, $e^{\pm}$, ν_{μ}, $\mu^{\pm}$, ν_{τ}, τ
We emphasize that this list is but a fraction of the particles observed to date. fortunately, the properties of these particles suggest a pattern consistent with them in turn being made out of a "small" number of more elementary objects called quarks. To date, despite many attempts, there are no reliable reports of an isolated quark actually being observed.

Clearly, a theory is needed that explains the rich particle spectrum in terms of quarks and yet is compatible with quarks being unobservable if isolated from other matter. Further, from past experience with mathematical formulations, it is natural to insist that this description be reasonably simple and elegant. There is exactly one existing candidate for such a description. It is called Quantum Chromodynamics or Q.C.D. It is based on the very successful quantized description of the electromagnetic field interacting with electrons or Q.E.D. Q.C.D. is more complicated than Q.E.D. because the several species of quarks needed to explain the group structure of the observed particles as well as the confinement of single quarks allows for a very rich mathematical structure. This structure is carried in a partition function like object which is the exponential of an action made of qlue fields (designated by the symbol A and quark fields designated by the symbol ψ. Here we have suppressed the space time dependence of these fields as well as the fact that each symbol is actually a vector with at least 12 components. The interaction described by the action is highly non-linear but any term contains either zero or two quark fields which somewhat simplifies the formulation. The primary content of the assumption that system examined be a quantum field theory is that at any given time every point in space has assigned to it independent quantized degrees of freedom associated with the qlue and quark fields. It is thus very natural to describe space time mathematically as a discrete lattice of points with separation a that approaches zero.



The object U(i,j) defined as

$$U(i,j) = e^{i g_0 A \cdot (\vec{i} - \vec{j})}$$

plays a primary role in this theory. It has the property that $U(i,j) = U^{\dagger}(j,i)$. Further the $U(i,j)$ are members of the qroup of unitary unimodular matrices SU(3). For these fields alone we have

the (effective) partition function

$$W = e^{S_g}$$

Here $$S_g = \frac{1}{g_c^2} \sum S_\square$$

where the sum is taken over all independent square plaquettes and

$$S_\square = tr[U(i,j)U(j,k)U(k,l)U(l,i)]$$

We could stop with this form for the partition function and have more work to do than current available machine power will allow. However, to calculate the elementary particle spectrum (except for glueballs) we must include the quark fields in our action. The form used because of various symmetry and guage principles is

$$S_f = -\sum_i \bar{\psi}(i)\psi(i) + K\sum_{i,j} \bar{\psi}(i)B(i,j)\psi(j)$$

Here K is a numerical parameter. The matrix B depends explicitly on the glue field A (of course leaving out gravity and weak interactions) S_f is then taken to be

$$S = S_f + S_g$$

Physics is obtained by calculating the correlation functions or vacuum expectations of polynomials of the field (quark and glue) of the partition function formed from this action. The general problem that must be confronted is the evaluation using the appropriate group measure of the following type of integral.

$$\langle P(\psi,\bar{\psi},U)\rangle \propto \int [\Pi\, dU][\Pi\, d\bar{\psi}\, d\bar{\psi}]\, P(\psi,\bar{\psi},U)\, e^{S}$$

This has many variables . Since each U(i,j) is an SU(3) matrix it is specified by 12 numbers. If we study a hypercubic lattice with N points in each space-time direction we are dealing with the order of N**4*12*4 numbers just associated with the glue fields. The quark fields are characterized by (for our discussion) 12 complex numbers at each lattice point. However, this is just the beginning. The quantities are in fact not numbers! They have the property that $\psi(i)\psi(j) = -\bar{\psi}(j)\psi(i)$. This anticommutivity property is essential in order that the quarks describe objects with intrinsic half integral spin. Because the action S is quadratic only in quark fields it is possible (using very natural

definitions) to explicitly perform the integration over quark fields and leave the problem of evaluation of correlation functions expressible entirely in terms of integrals over glue fields. For example, if we examine the correlation function of four quark fields we have $<\bar{\psi}(a)\psi(b)\bar{\psi}(c)\psi(d)>=$

$$-\int[\Pi dU]\left[(1-KB)^{-1}_{bc}(1-KB)^{-1}_{ad}\det(1-KB)e^{S_g}\right]$$

Note that 1-KB is a (N**4*12)**2 complex matrix. Det(1-KB) is more or less unspeakable for any reasonable size of N. Evaluation of the correlation function above is essential for determining meson masses (such as the pion) in this theory. Calculation of correlations of expectations of six quark fields is needed to evaluate properties of baryon fields (such as the proton). As a practical matter, numerical evaluation of six quark correlations is not much more difficult than four quark correlations. Clearly as N gets larger the problem gets more complicated. However, we are really only interested in the limit when N is very large since this corresponds to the infinite physical world. Indeed, we want to examine the limit were N becomes infinite and the lattice spacing a approaches zero. Under some circumstances it can be argued that neglecting the determinant should not make dramatic changes is the nature of the physical answers we obtain. For this discussion (and the particular project it is outlining) we chose to set the determinant to unity. We are then left with a class of integrals to evaluate which can be handled using Monte Carlo importance sampling methods in conceivable amounts of time for reasonably big lattices. Such systems have been studied extensively using Vax (780) computers on lattices with 6**3*14 points. Using the C.S.U. Cyber 205 it is possible to examine far larger systems. Indeed we are in the process of examining (on several class 6 computers) systems with 10**3*24, 12**3*32 and 20**3*50 lattice sites.

After neglecting the determinant we are left with the basic structure

$$<\bar{\psi}(a)\psi(b)\bar{\psi}(c)\psi(d)>\sim -\int[\Pi dU]\left[(1-KB)^{-1}_{bc}(1+KB)^{-1}_{ad}e^{S_g}\right]$$

We evaluate this numerically in two steps. First, we define a probability

$$dP(U)\equiv\frac{1}{Z}e^{S_g}\,dU$$

Using Monte Carlo (Metropolis) methods we generate a sequence of glue configurations which are are distributed according to $dP(u)$. It is important that these distributions be thermalized and "statistically independent". By careful tuning of the way the Monte Carlo hits are made taking into consideration the nature of the group measure we can enormously speed up the decorrelation of consecutive lattice configurations. Indeed for most cases, it is not difficult to obtain a factor of four increase in speed of lattice generation over conventional methods through careful tuning. Even careful tuning of the physics of this problem does not give reasonable run times for large lattices unless full advantage is taken of the possibility of vectorizing the code. To do this efficiently we use red black methods of sweeping through lattice configurations. In addition, the memory requirements for large lattices rapidly become excessive so we use time slicing to control our memory allocations. We must do this since the demand paging algorithm on the 205 does not work efficiently with the codes which are naturally written for this problem.

After a collection of independent lattices are generated we continue to evaluate the basic integral for the problem by evaluating the inverse of 1-KB for the guage configurations of each lattice. This is somewhat simplified since this inverse need be evaluated for only one base site-that is a fixed row of the matrix. However, it turns out that this inversion must be carried out for three or four different values of the parameter K. The method that has been most commonly used to invert the matrix employs a Gauss Seidel method. This is slow, taking almost an order of magnitude more time than the lattice generation. We have other methods under study which for the particular systems involved promise to be much faster. The Gauss Seidel method is used in a form first applied to this problem by Weingarten. We need to evaluate the form

$$f = (1 - KB)^{-1} h$$

Here h is at a fixed lattice point but can vary through the 12 values associated with the indices of the quark field at that point. This equation is now re-written in the form

$$f = h + KBf$$

$$\Rightarrow f = h + KBf + (1-\lambda)(f - h - KBf)$$

$$= (1 - \lambda + \lambda KB) f + \lambda h$$

λ is a parameter which can be tuned in order to obtain the

fastest convergence in the solution of this equation by iteration in f. In practice we code this procedure using red black ordering and time slicing to obtain vectorization and efficient memory management.

After the matrix inversion is performed and the correlations are evaluated through weighting over the available lattices we must extract physical information from the output functions. The easiest information obtained is the masses of the particles described by this formalism. It is ,for example, a general property of the theory that we are dealing with that if we look at correlation functions depending on only two space time points and then sum over all spatial directions that the resulting time dependent functions depend only on sums of exponentials with the exponent linear in the masses of the appropriate particles and the time separations. It is an easy matter to fit to exponentials and extract numerical values for the masses. However to do this we must tune the parameters of the theory to match the physical mass spectrum at some value of the mass. In effect we have a two parameter fit for the entire mass spectrum. It is found however that the Gauss Seidel method fails to converge for the physical value of the pion mass and hence the need to do the extrapolation in K mentioned earlier. After this is done, it has been found that on smaller lattices a fairly accurate fit can be obtained to the relatively light particles. We expect to find much better fits for a large lattices where edge effects should ha ve a smaller effect on the calculated results.

REFERENCES

Many workers have contributed to this new field. Without any attempt to be complete we list some references which will give the the interested reader a starting point for study of the topics discussed in this talk.

1. K. Wilson, Phys. Rev. D10, 2445 (1974)
2. M. Creutz, L. Jacobs and C. Rebbi, Phys. Rev. D20, 1915 (1979)
3. M. Creutz, Phys. Rev. D21, 2308 (1980)
4. D. Weingarten, Nucl. Phys. B215¢fs7*, 1 (1983).
5. F. Fucito, E. Marianari, G. Parisi, and C. Rebbi, Nucl. Phys. B180, 369 (1981).
6. W. Duffy, G. Guralnik, and D. Weingarten, Phys. Lett 125B,311, (1983)